Hybrid Particle-Continuum Computations of Nonequilibrium Hypersonic Flows

Iain D. Boyd and Wen-Lan Wang
Department of Aerospace Engineering
University of Michigan, Ann Arbor, MI 48109
Ann Arbor, MI 48109

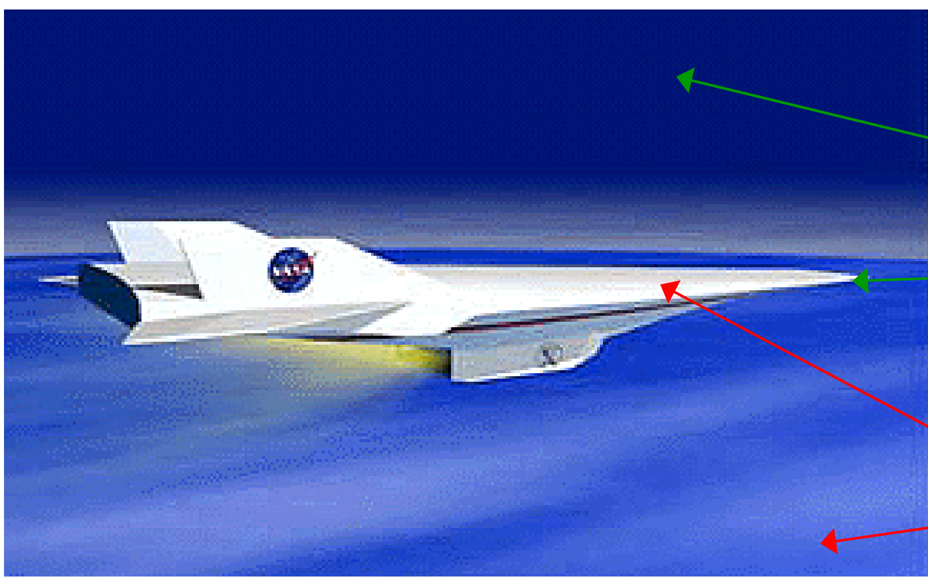
Supported by AFOSR and NASA

Overview

- Background and motivation.
- Numerical schemes:
  - CFD/DSMC-IP hybrid approach;
  - domain coupling;
  - location of interface.
- Hypersonic flow examples:
  - normal shock waves;
  - blunted cone tip.
- Summary and conclusions.

Background

- Hypersonic vehicles encounter a variety of flow regimes:
  - continuum: modeled accurately and efficiently with CFD;
  - rarefied: modeled accurately and efficiently with DSMC.
- A hybrid DSMC-CFD method is attractive for mixed flows:
  - CFD: Navier-Stokes finite-volume algorithm;
  - DSMC: MONACO+Information Preservation (DSMC/IP).



Rarefied DSMC approach:

based on kinetic theory

high altitude

sharp edges

Continuum CFD approach:

solve NS equations

low altitude

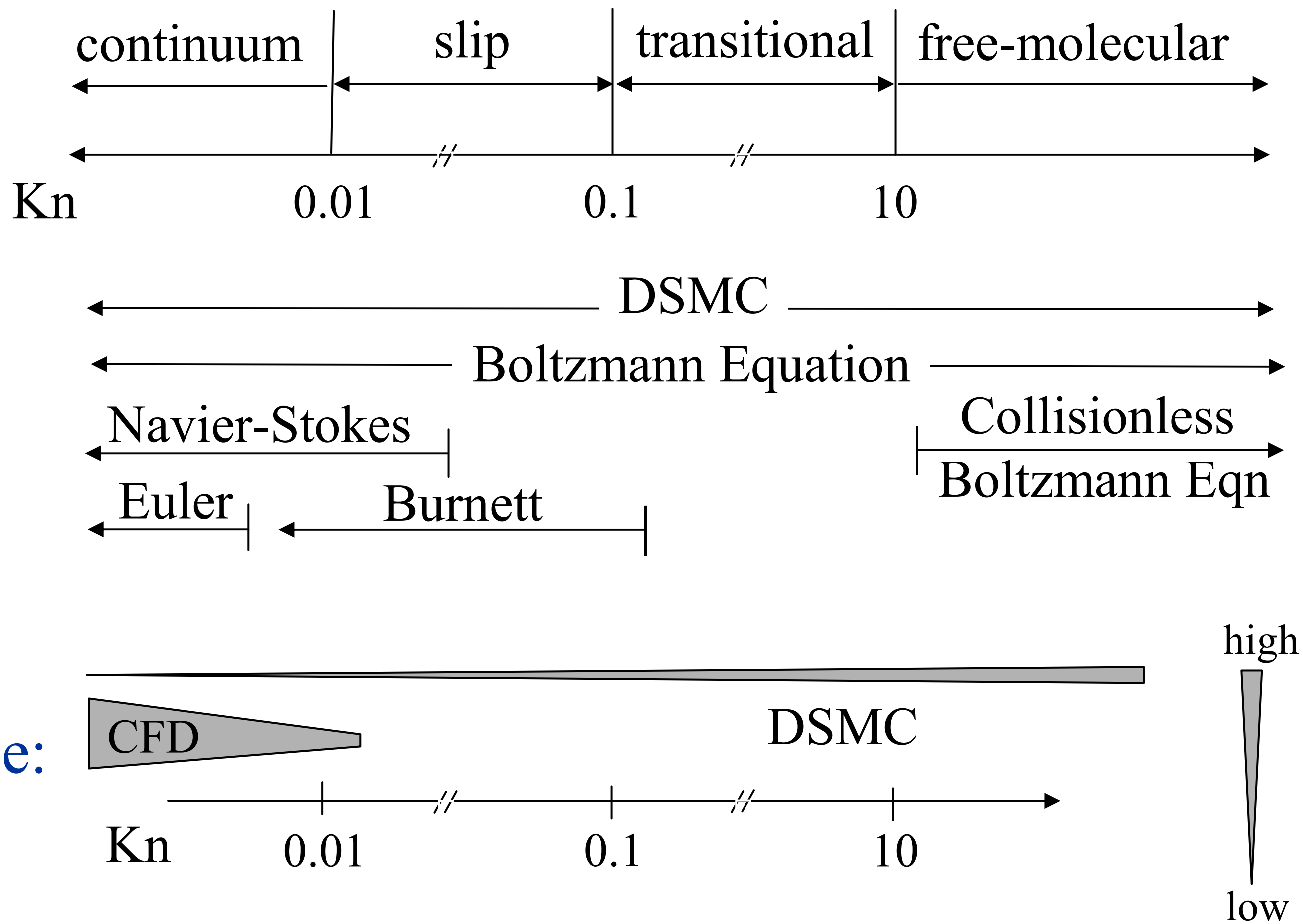
long length scales

Motivation for Hybrid Method

Flow Regimes:

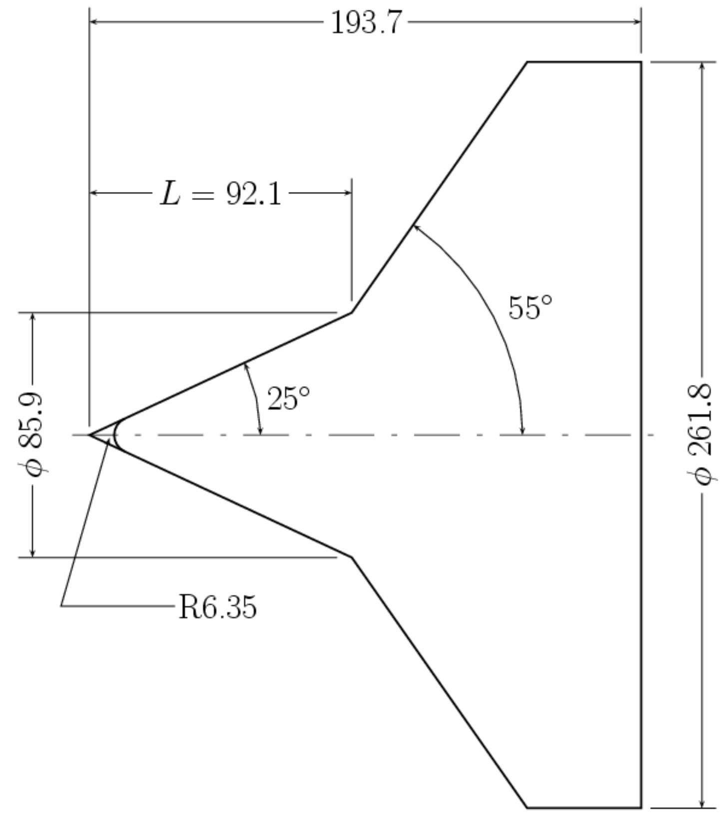
Model Accuracy:

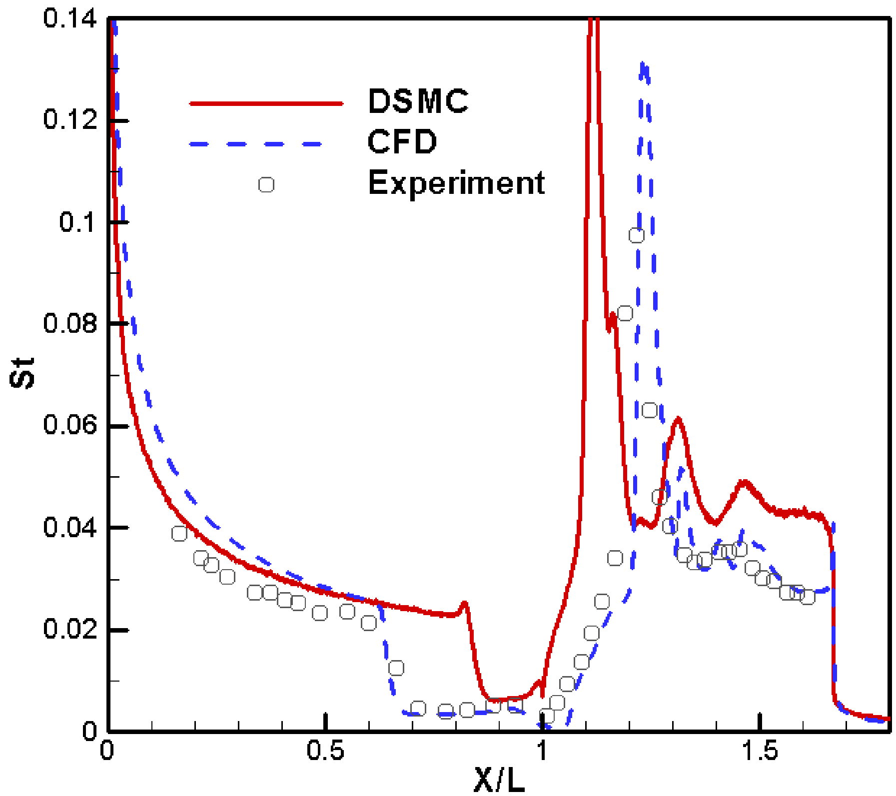
Numerical Performance:



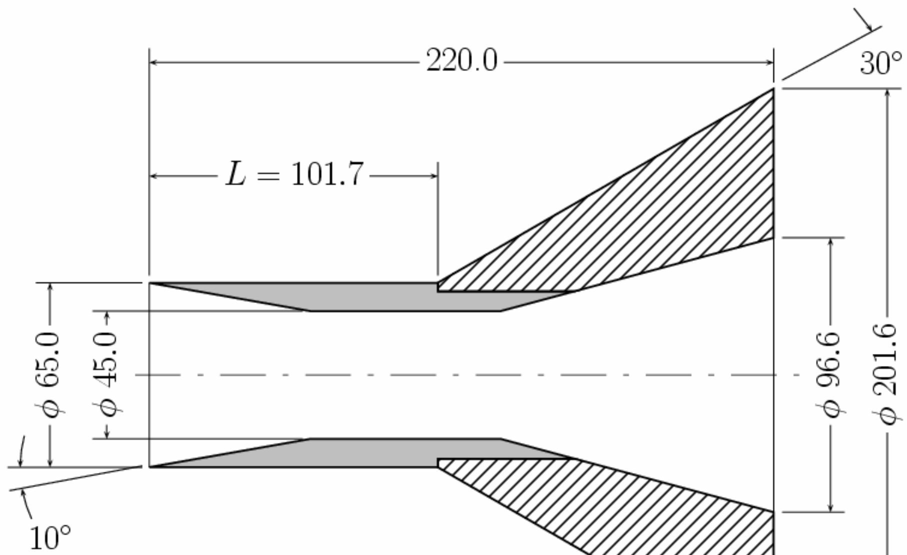
Accuracy
Performance } ⇒ hybrid approach

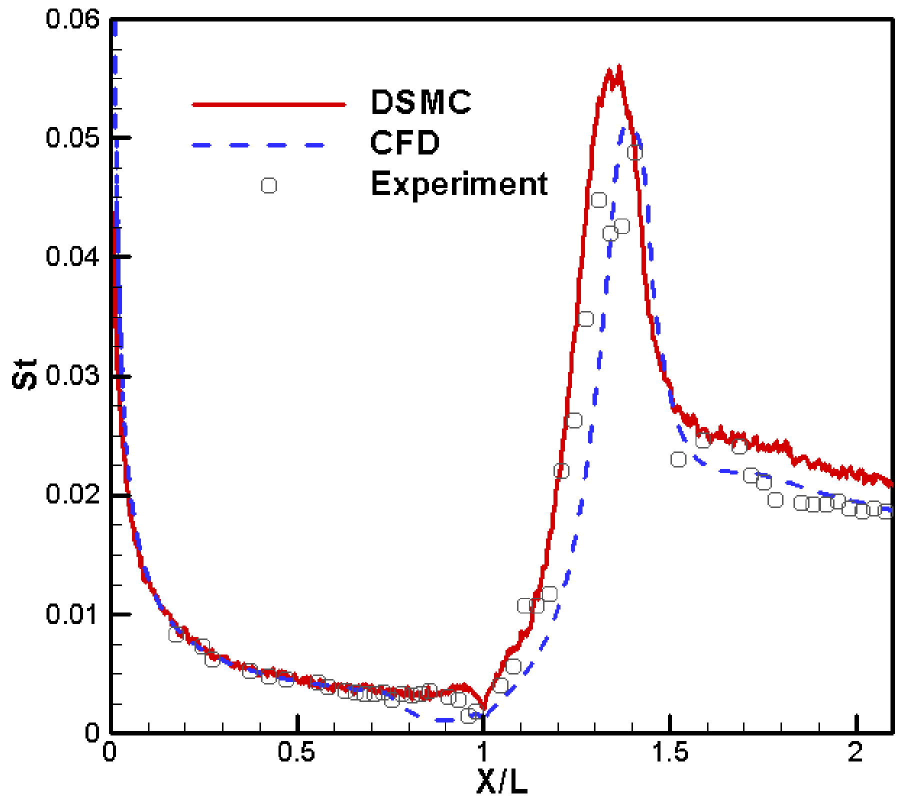
Example Where CFD Works Best





Example Where DSMC Works Best





Hybrid Approach

MacCormack and Candler
Comp. Fluids, **17**, 1989

Sun and Boyd
J. Comp. Phys., **179**, 2002

Navier-Stokes solver

interface

DSMC/IP method

2nd order accurate modified Steger-Warming flux-vector splitting approach (FVM)

Macroscopic properties are preserved as well as microscopic particle information

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial r_i}(\rho u_i) = 0$$

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial}{\partial r_i}(\rho u_{ij} + P_{ij}) = \frac{\partial}{\partial r_i}\tau_{ij}$$

$$\frac{\partial e}{\partial t} + \frac{\partial}{\partial r_i}[(e+P)u_i] = \frac{\partial}{\partial r_i}(u_j \tau_{ij} - q_i)$$

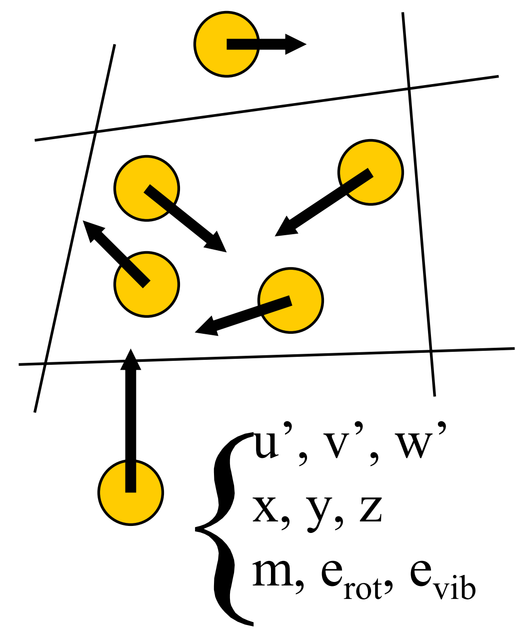
$$\frac{\partial \rho_c}{\partial t} + \frac{\partial}{\partial r_i}(\rho_c V_{i,c}) = 0$$

$$V_{i,c} = \frac{1}{N_p}\sum_{j=1}^{N_p} V_{i,j}$$

$$T_c = \frac{1}{N_p}\sum_{j=1}^{N_p}(T_j + T_{a,j})$$

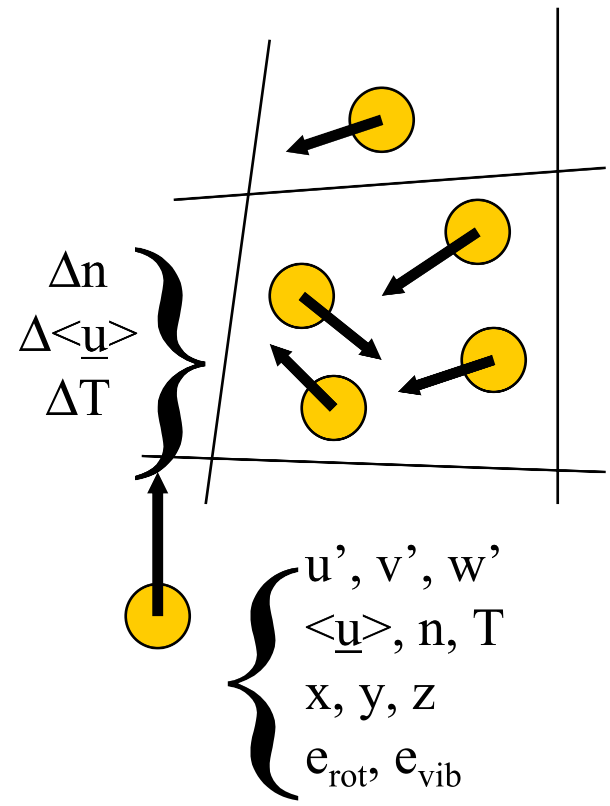
Direct Simulation Monte Carlo (DSMC)

- Particle method for nonequilibrium gas flows:
  - developed by Bird (1960's);
  - particles move/collide in physical space;
  - particles possess microscopic properties, e.g. u' (thermal velocity);
  - cell size $\Delta x \sim \lambda$, time step $\Delta t \sim 1/\nu$;
  - collisions handled statistically (not MD);
  - ideal for supersonic/hypersonic flows;
  - thermochemical nonequilibrium models.

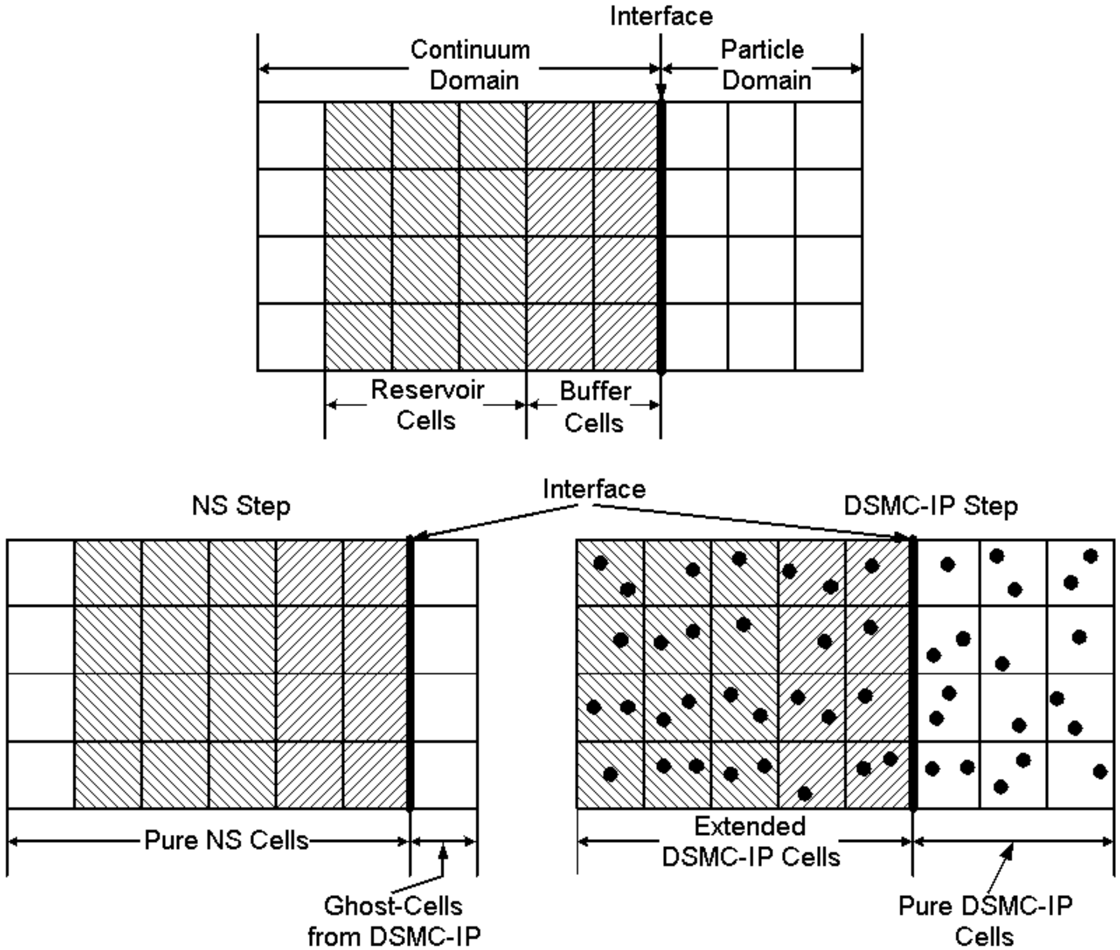


Information Preservation Method

- A novel particle approach for gas flows:
  - evolves alongside DSMC;
  - particles and cells possess preserved information, e.g. n, $\langle \underline{u} \rangle$, T;
  - Δn from number conservation;
  - $\Delta\langle \underline{u} \rangle$ from momentum conservation;
  - ΔT from energy conservation;
  - greatly reduces statistical fluctuations;
  - provides DSMC-CFD interface.



Domain Coupling



Interface Location: Continuum Breakdown Parameters

- Local Knudsen number, hypersonic flow (Boyd et al., 1995)

$$Kn_{GLL-Q} = \frac{\lambda}{Q}\left|\frac{dQ}{dx}\right| > 0.05$$

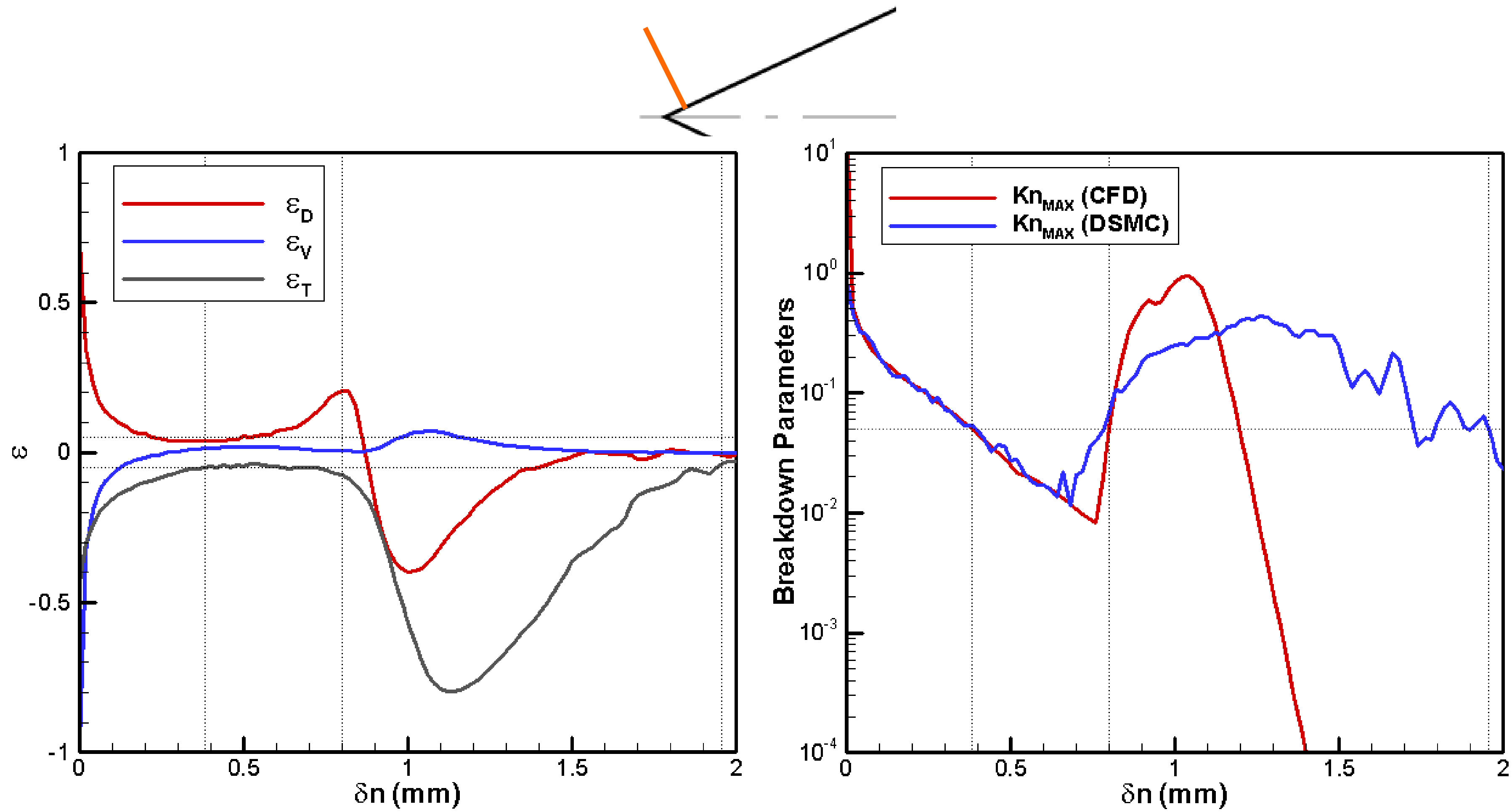
  - where Q= ρ, T, V.

- Determined through detailed DSMC versus CFD comparisons:

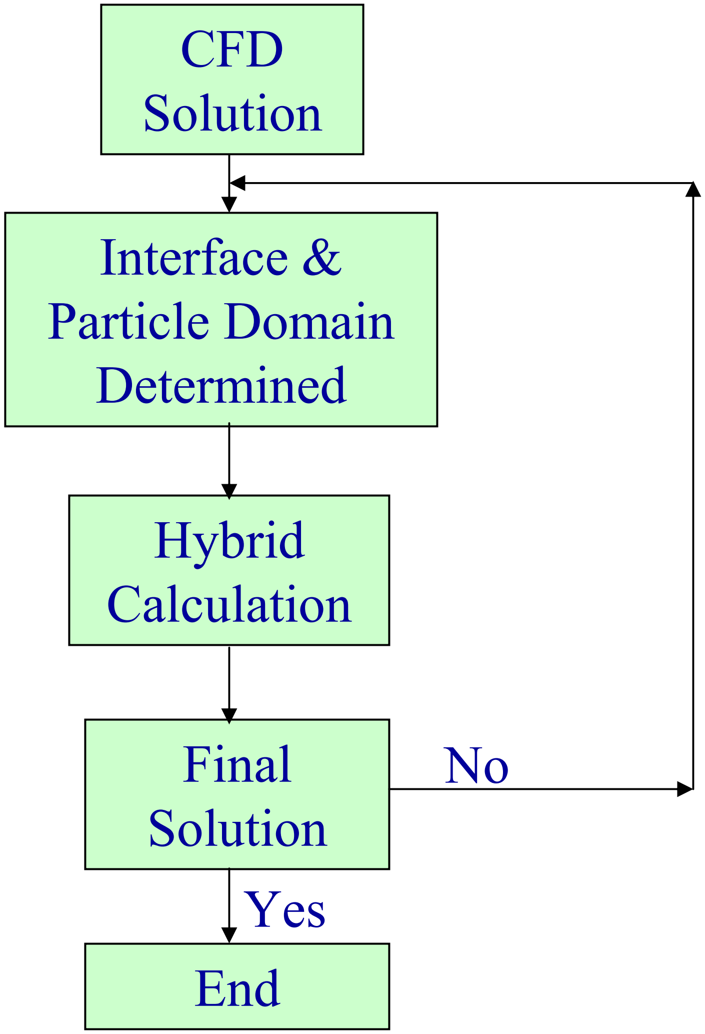
$$\mathrm{Kn}_{\mathrm{max}} = \max(\mathrm{Kn}_D, \mathrm{Kn}_V, \mathrm{Kn}_T)$$

- Parameters also under investigation for use inside DSMC:
  - failure of breakdown parameters at shock front;
  - use DSMC to evaluate *continuum onset* parameter?

Cut-off Value = 0.05



Hybrid CFD/DSMC-IP Process



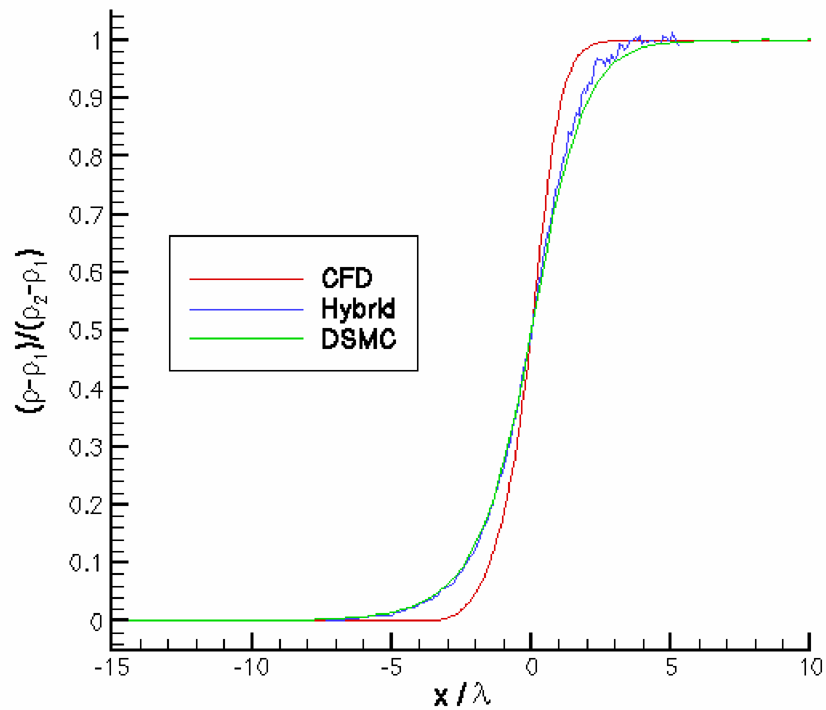
Summary of Hybrid Code

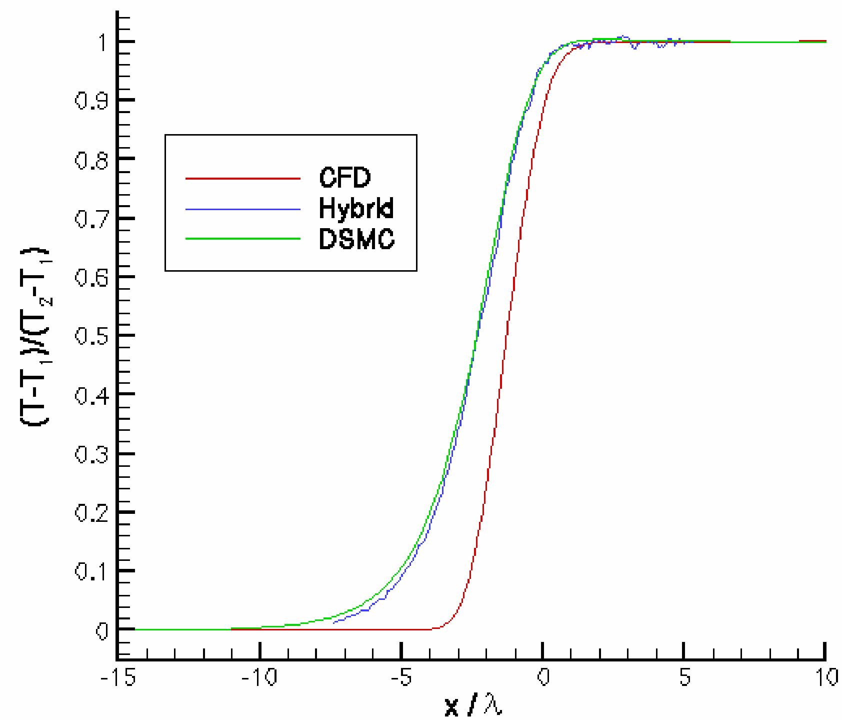
- Numerical methods:
  - 2d/axially symmetric, steady state;
  - CFD: explicit, finite volume solution of NS Eqs.;
  - DSMC: particle simulation;
  - interface: Information Preservation scheme;
  - implementation: a single, parallel code.
- Physical modeling:
  - simple, perfect gas (rotation, but no vibration);
  - walls: slip / incomplete accommodation;
  - breakdown parameter: local Knudsen number.

Numerical Example (1)
Normal Shock Waves of Argon

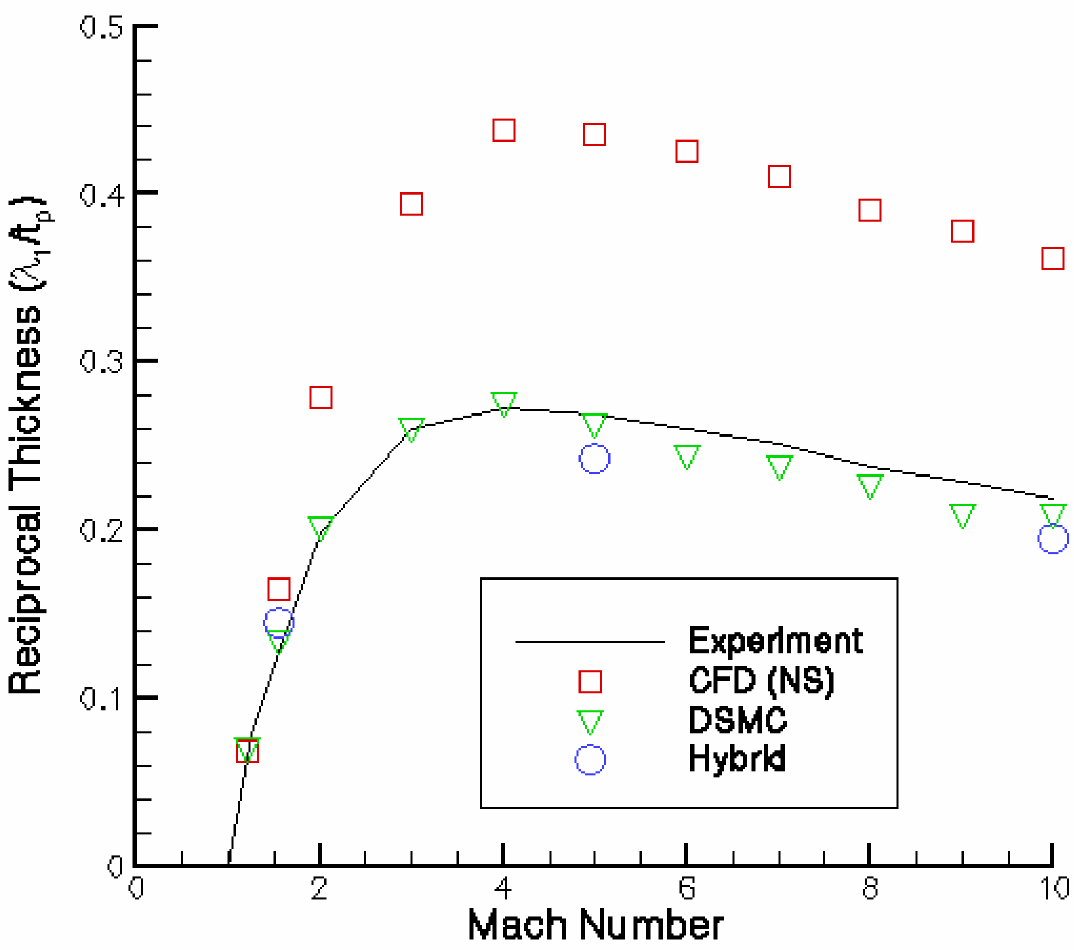
- Argon normal shocks investigated:
  - relatively simple hypersonic flow;
  - Alsmeyer experimental measurements;
  - well-known case for testing new algorithms.
- Simulations:
  - modeled in 2D (400 x 5 cells);
  - initialized by jump conditions;
  - pure DSMC;
  - pure CFD (Navier-Stokes equations);
  - hybrid code initialized by CFD solution.

Mach 5 Profiles





Reciprocal Shock Thickness

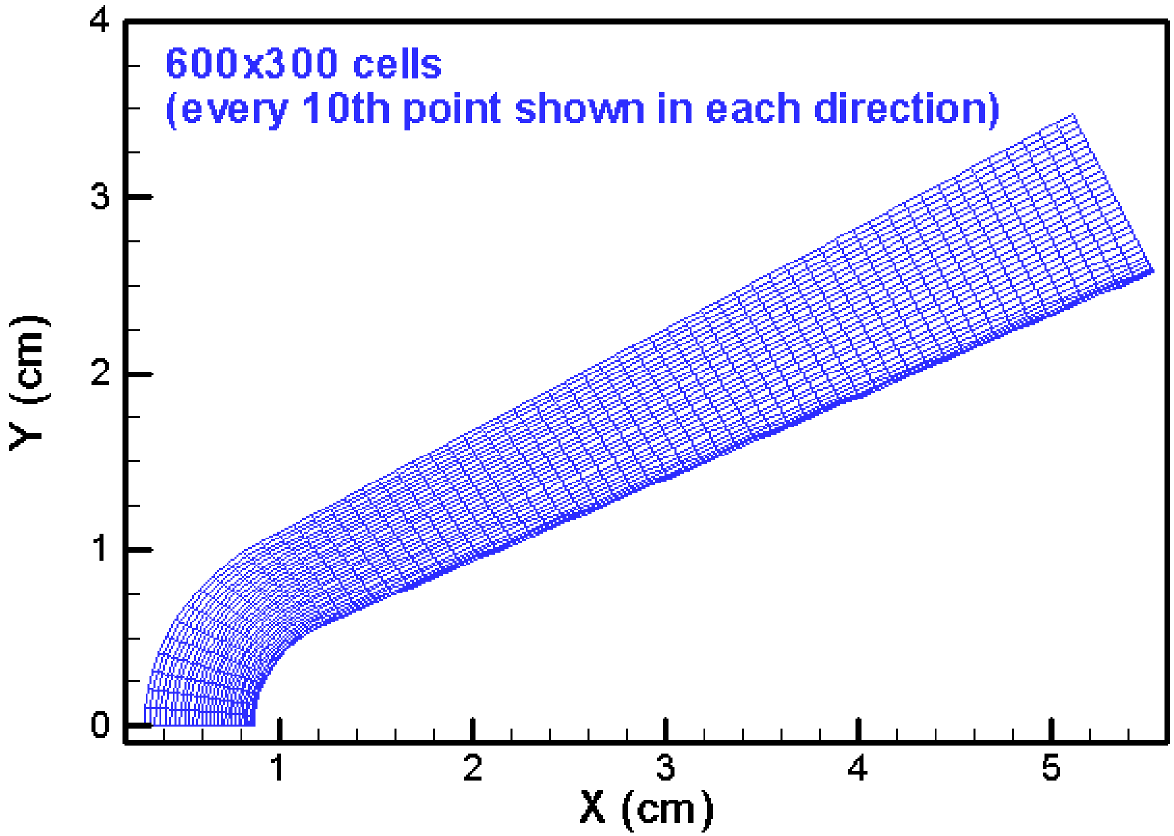


Numerical Performance

Method	CPU Time (sec) Per Iteration
Pure CFD	0.032
Pure DSMC	0.48
Hybrid	0.29

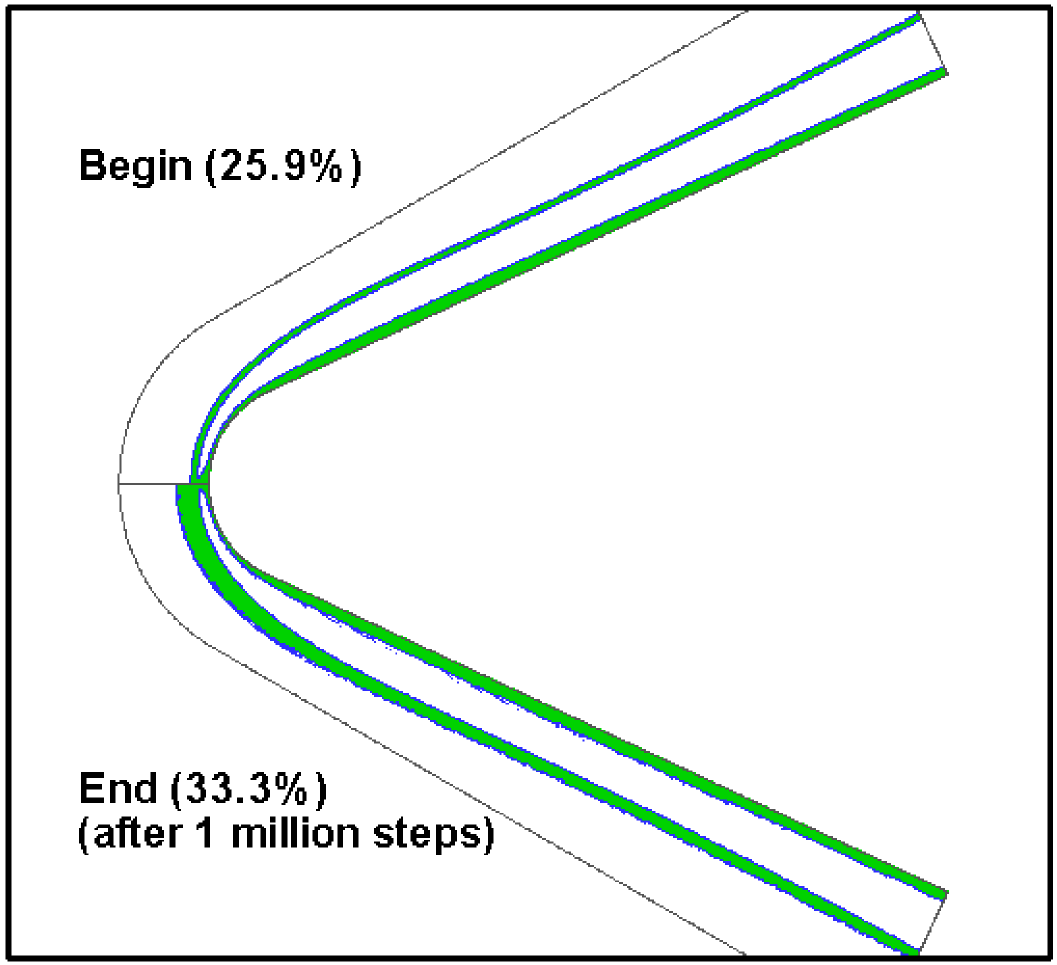
- Hybrid simulation employed 57% particle cells
- DSMC time-step could be 20 times larger

Numerical Example (2)
Blunted Cone

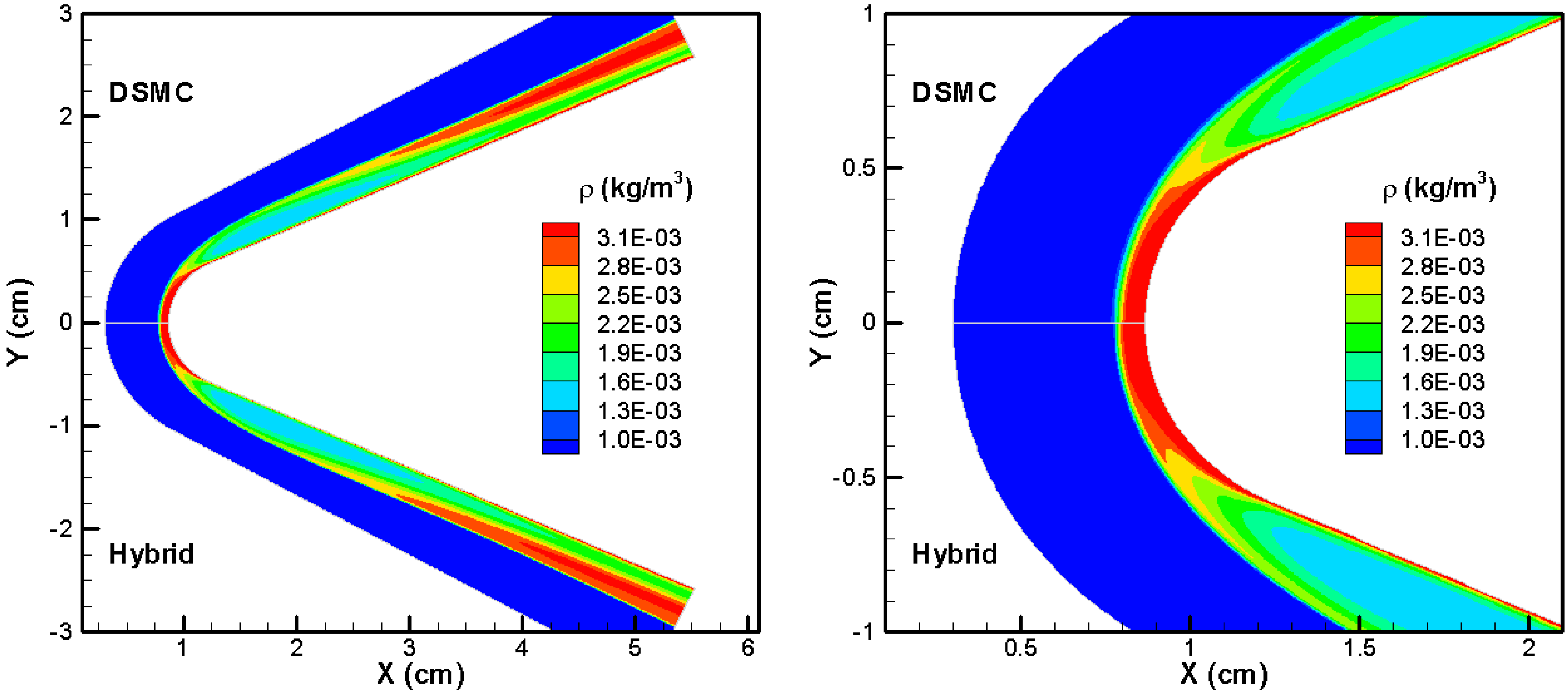


Ma_∞	λ_∞ (m)	ρ_∞ (kg/m^3)	U_∞ (m/s)	T_∞ (K)	T_{vib} (K)	T_w (K)
12.6	1.28×10^{-4}	5.618×10^{-4}	2630.4	104.4	2680.2	297.2

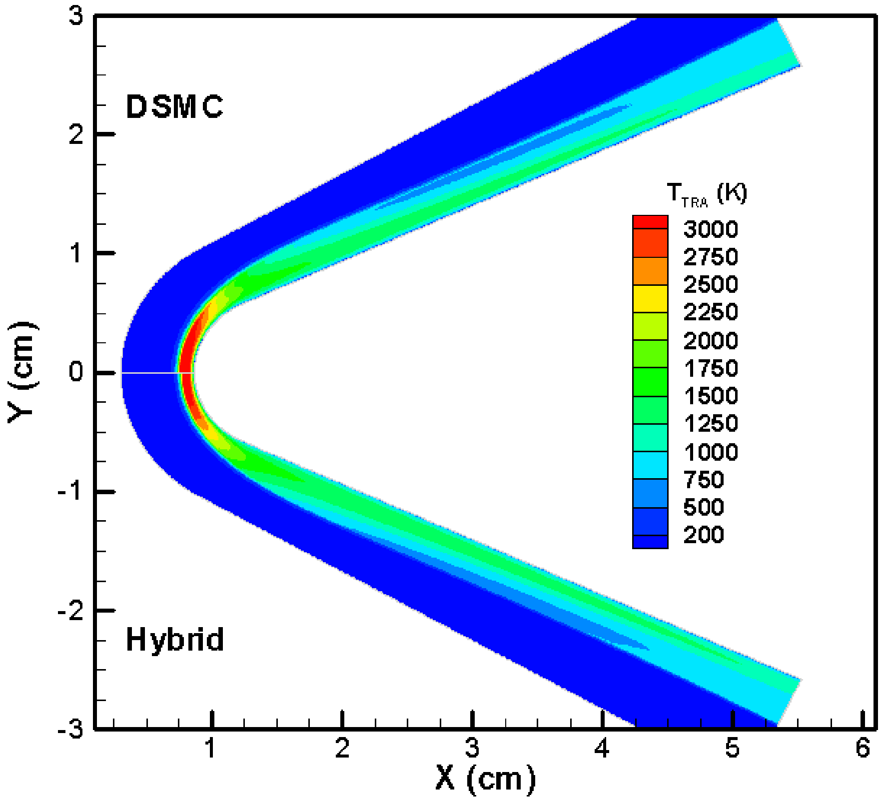
Particle Domain ($Kn_{max} > 0.03$)

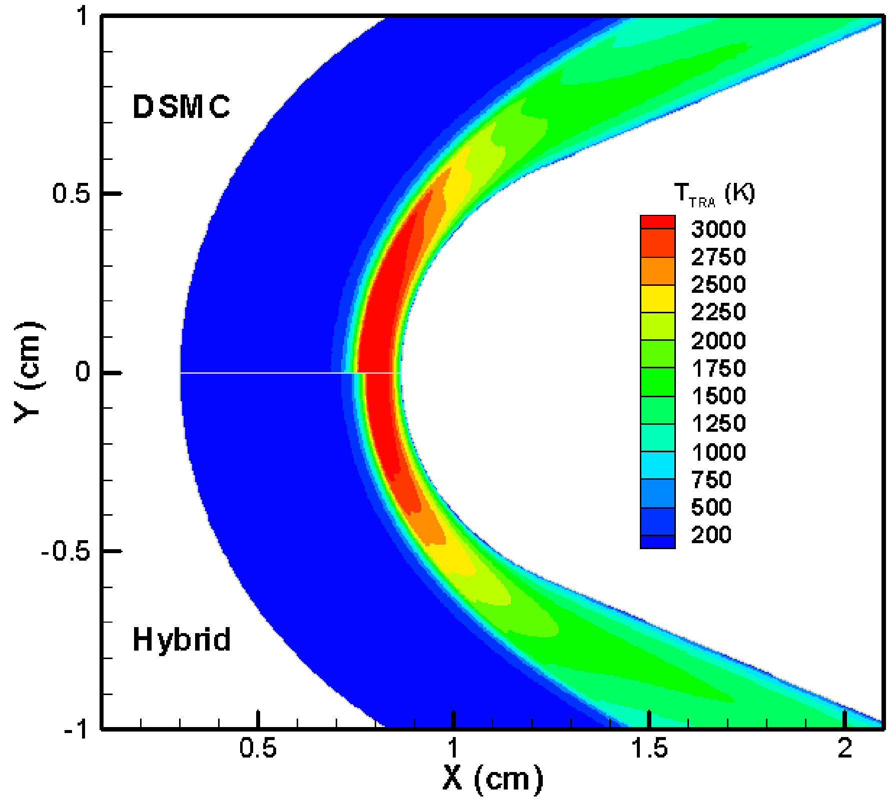


Comparisons of Density Contours

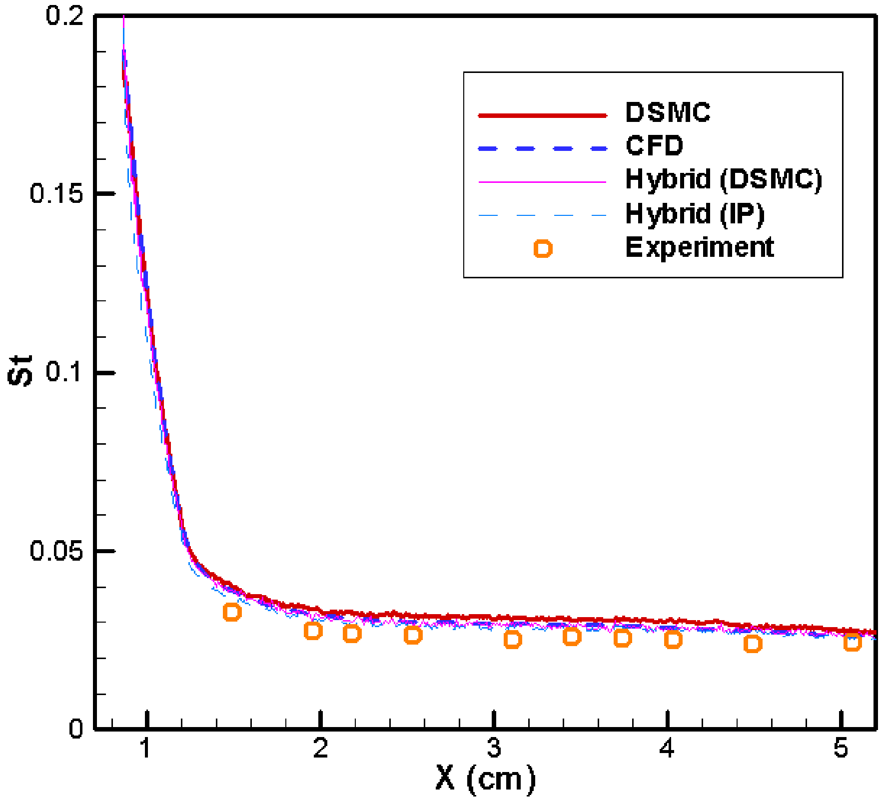


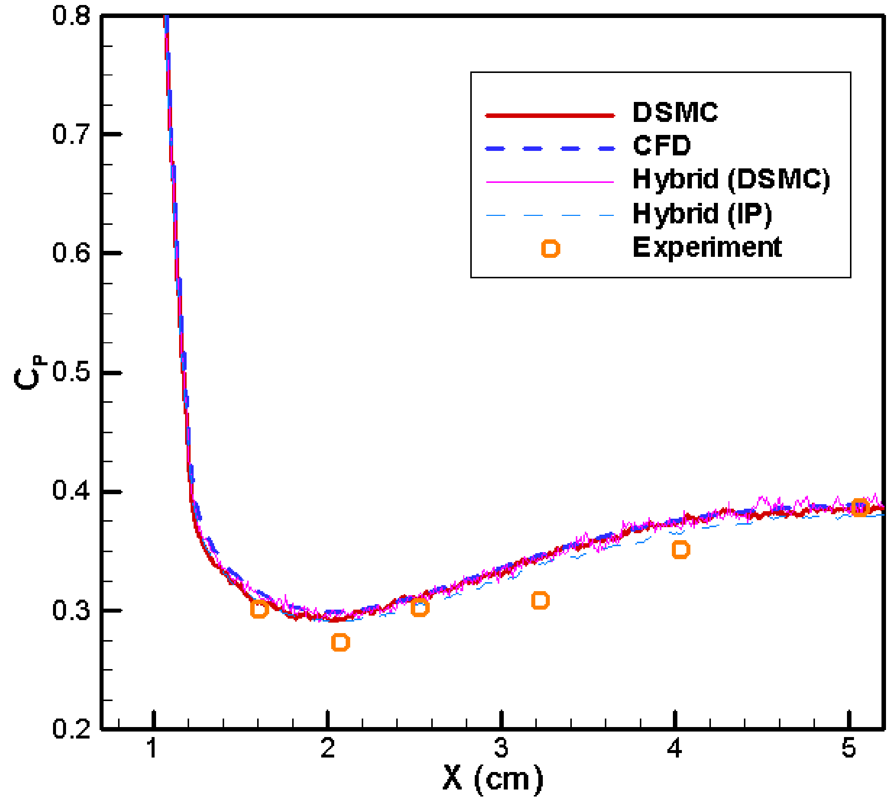
Comparisons of Temperature Contours



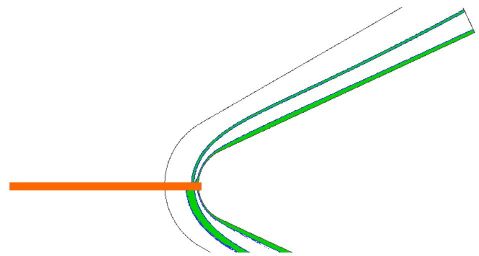


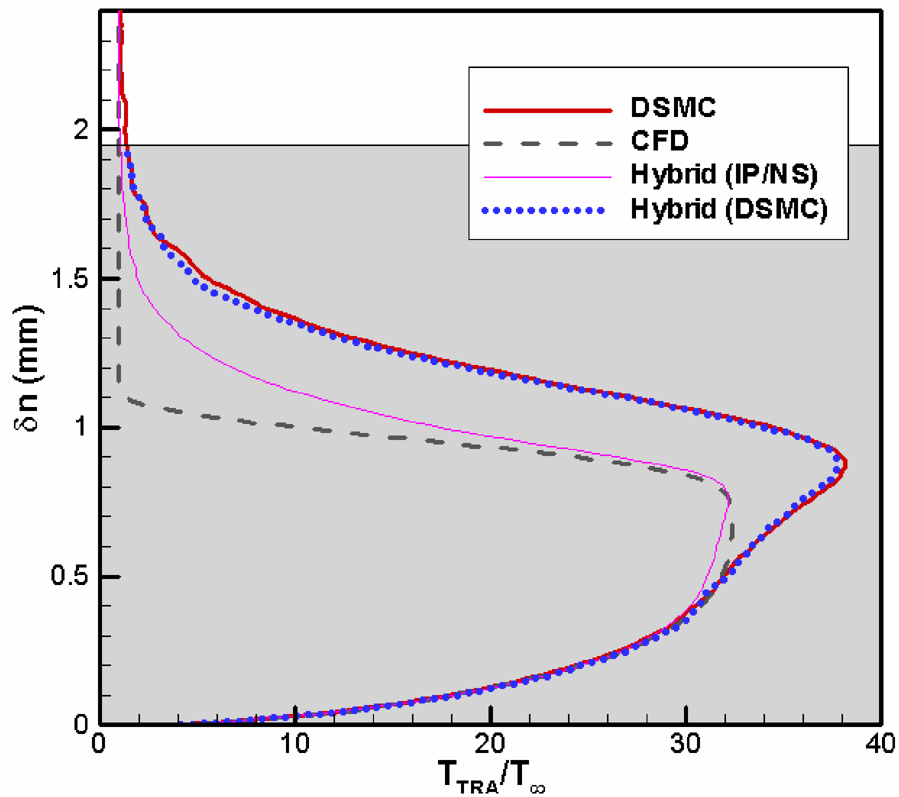
Comparisons of Surface Properties

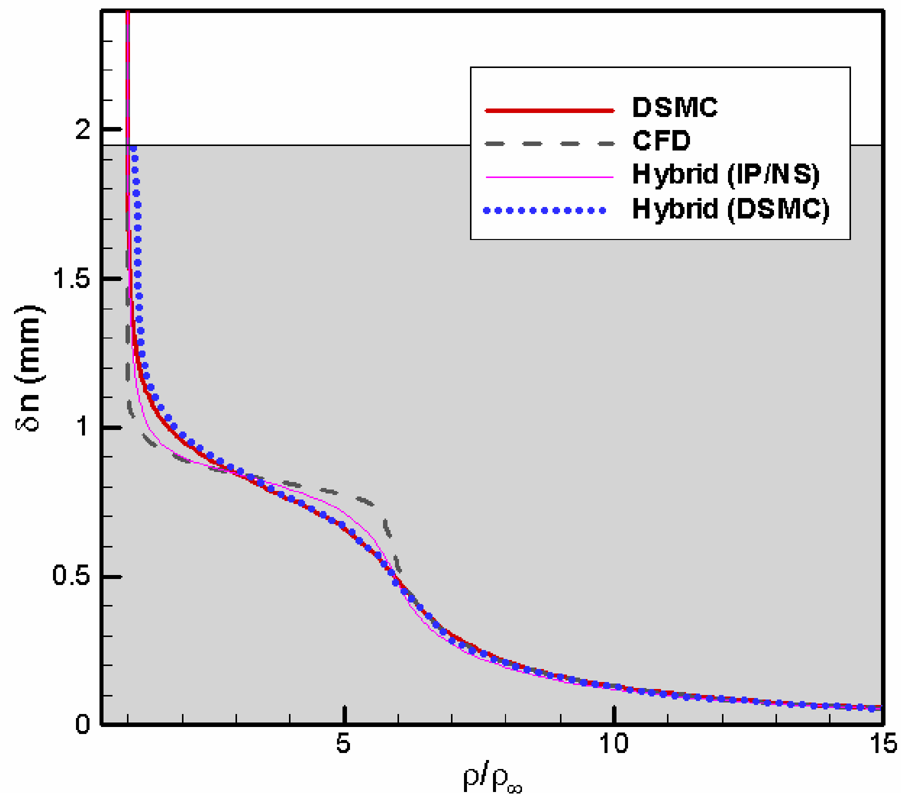




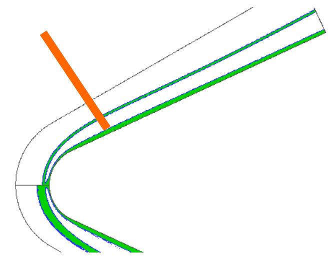
Detailed Comparisons Along the Stagnation Streamline

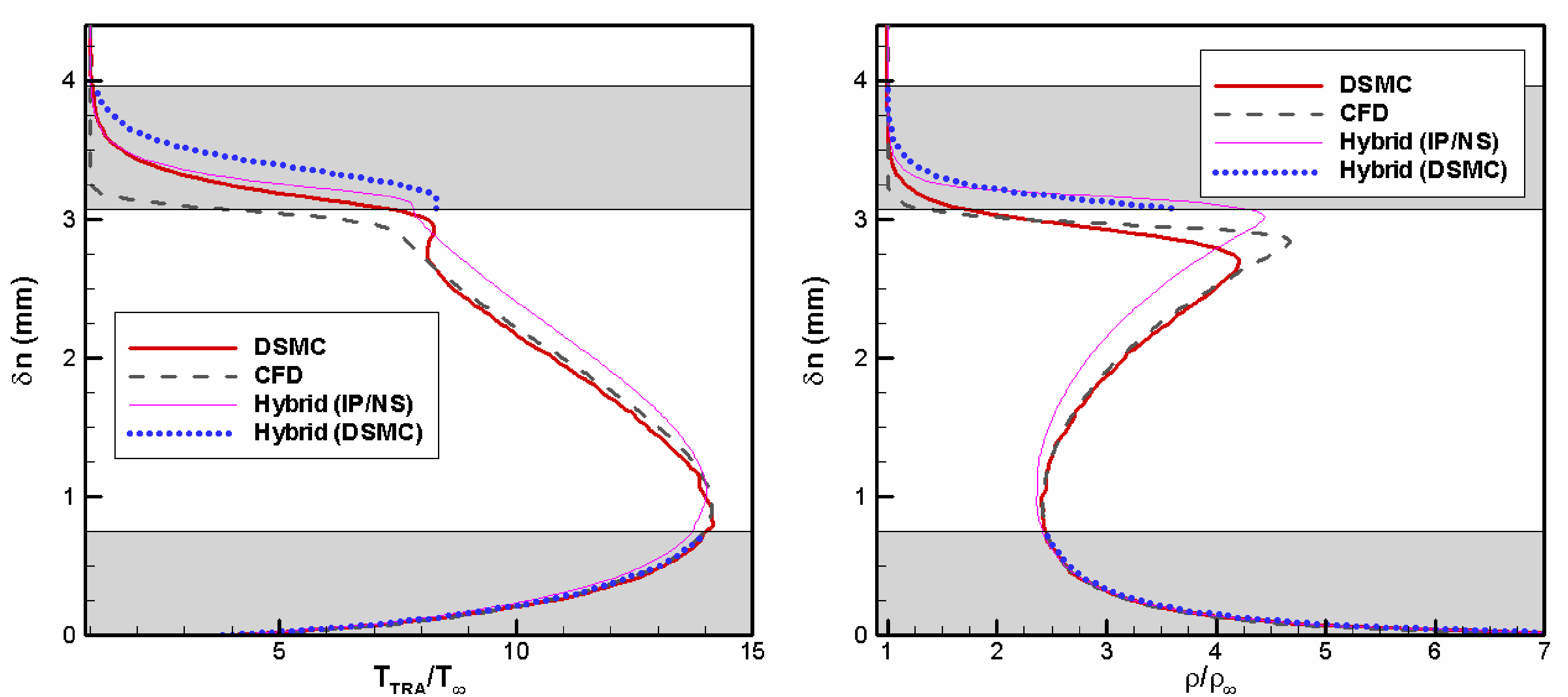




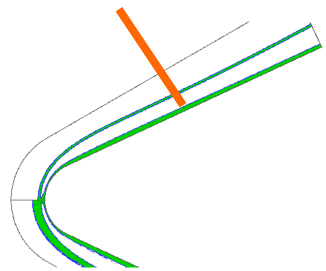


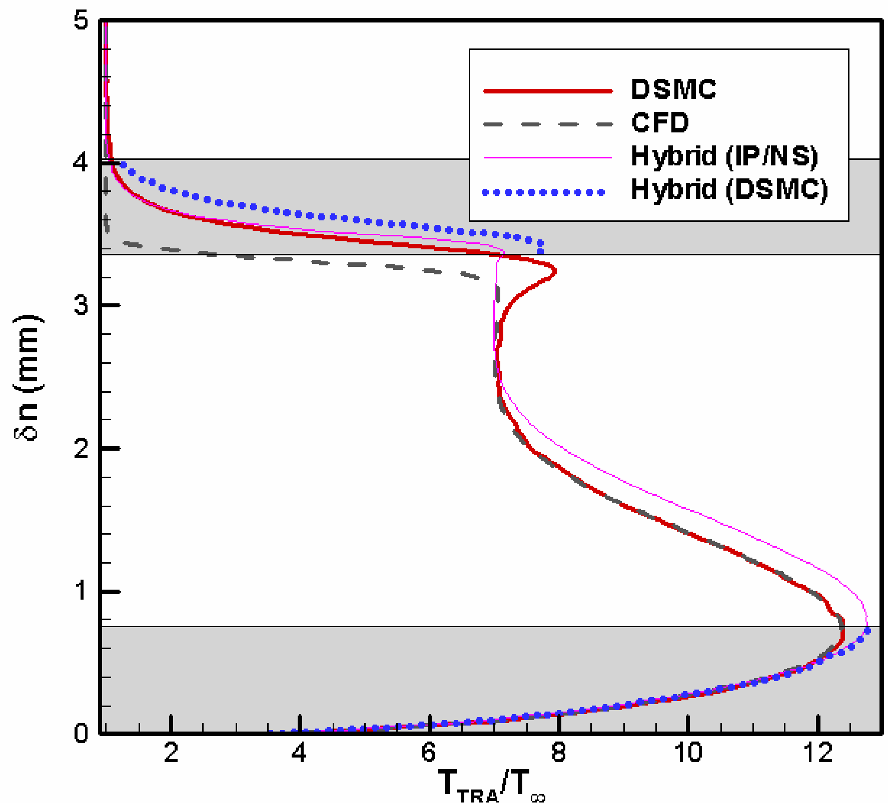
Detailed Comparisons at x = 2 cm

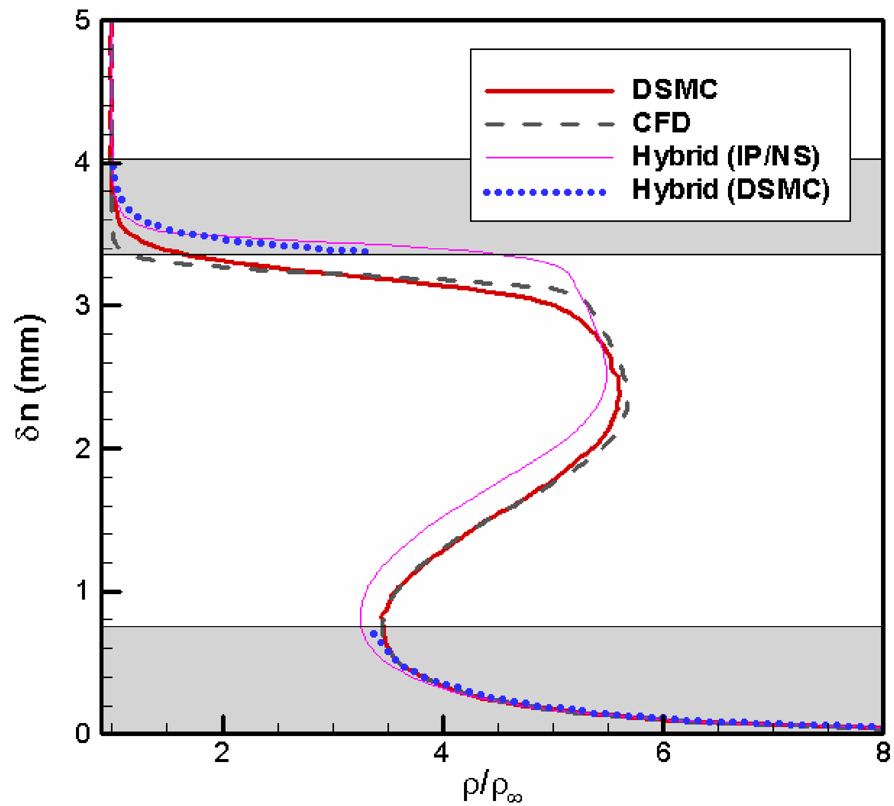




Detailed Comparisons at x = 4 cm







Summary

- Hybrid continuum-particle algorithm developed:
  - based on NS and DSMC methods coupled using IP;
  - 2d/axially symmetric;
  - perfect gas physical model;
  - high-speed flow conditions tested;
  - fully parallelized using MPI.
- Assessment of hybrid methodology:
  - able to compute shock waves and complex hypersonic flows;
  - able to move CFD solution to DSMC solution;
  - need to improve continuum interface prediction;
  - need to greatly improve numerical performance.

Future Directions

- Algorithm development for hybrid method:
  – CFD: parallel, implicit solver on unstructured mesh;
  – DSMC: implicit and/or other acceleration schemes.
- Physics development for hybrid method:
  – vibrational relaxation;
  – chemically reacting gas mixture.
- Development of hybrid methodology:
  – refinement of breakdown parameters;
  – evaluation against data (measured, computed).